Indian J. Phys. **44**, 244–252 (1970)

Exact partition function of Ising model in magnetism in one, two and three dimensions in nonzero field

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(*Received* 16 *March* 1970)

Exact partition function has been obtained for Ising model in one, two and three dimensions in nonzero field and it is shown that transition temperature and spontaneous magnetization do not exist according to our exact calculations with this model.

Introduction

It is well known that Ising model (Ising 1925) in one dimension is not ferromagnetic. Two dimensional problem has been solved exactly (Onsager 1944), for non zero field) and also by approximate methods. Approximate calculations have also been carried out in three dimensions (Newell 1953). Two and three dimensional investigations lead to a transition temperature and spontaneous magnetization. Various types of lattice in two dimensions have also been considered. Here the problem has been solved for the linear chain, the two dimensional rectangular net and three dimensional rectilinear parallelopiped lattice as shown in figures 1–3. The results (free energy etc.) of one dimension should follow as a special case of those of two dimensions. Suppose in one dimension we have got one row with L sites. In two dimensions we have M rows and L columns. If $M = 1$, one dimension becomes a special case of two dimensions and two dimensional case should be a special case of three dimensions.

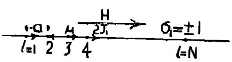


Fig. 1

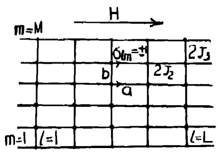


Fig. 2

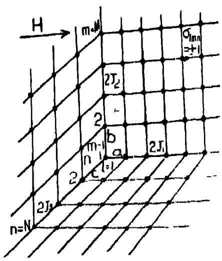


Fig. 3

Formulation of the model

A solid consists of crystals. All the crystals behave exactly in the same manner. Inside the crystal along X-axis there are L equidistant sites, the distance between two nearest neighbours being a, along Y axis there are M equidistant sites, the neighbouring distance being b, along the Z axis there are N equidistant sites separated by a distance c. For one dimension $M = N = 1$ and for two dimensions $N = 1$. In a magnetic field in each site the spin can have two orientations only, $+1$ and -1. Interaction between two neighbouring spins along X axis is measured by $2J_1$, along Y axis by $2J_2$, and along Z axis by $2J_3$. In one dimension $J_2 = J_3 = 0$ and in two dimensions $J_3 = 0$. We consider only the nearest neighbour interaction. We represent the spin of the (l, m, n)th site by σ_{lmn} and $\sigma_{lmn} = \pm 1$. The crystal symmetry is defined by $\sigma_{L+lmn} = \sigma_{lmn}$, $\sigma_{lM+mn} = \sigma_{lmn}$ and $\sigma_{lmN+n} = \sigma_{lmn}$. Inside a crystal no site is to be preferred to another site. Statistically all the sites are equivalent. Consider the arbitrary (l, m, n)th site anywhere in the crystal. In one dimension it will have interaction with two nearest neighbours, in two dimensions with four nearest neighbours and in three dimensions with eight nearest neighbours. Energy of lth site in one dimension will be given by

$$E_l = -\mu H\sigma_l - J_1\sigma_l\sigma_{l+1} - J_1\sigma_l\sigma_{l-1} \qquad \ldots (1)$$

with $\sigma_l = \pm 1, \quad \sigma_{l+1} = \pm 1$ and $\sigma_{l-1} = \pm 1$.

Here μ is magnetic moment per site and H is magnetic field. This will result in eight $(= 2^3)$ values of energy :

$$-\mu H - J_1,\ -\mu H,\ \mu H - J_1,\ \mu H,\ -\mu H,\ -\mu H + J_1,\ \mu H \text{ and } \mu H + J_1.$$

In two dimensions the arbitrary (l, m)th site will have energy given by

$$E_{lm} = -\mu H\sigma_{lm} - J_1\sigma_{lm}\sigma_{l+1m} - J_1\sigma_{lm}\sigma_{l-1m} - J_2\sigma_{lm}\sigma_{lm+1} - J_2\sigma_{lm}\sigma_{lm-1} \qquad \ldots (2)$$

The thirty two $(= 2^5)$ values of energy will be given by

$\mu H + 2J_1 + 2J_2$, $\mu H - 2J_1 + 2J_2$, $\mu H + 2J_2$, $\mu H + 2J_2$, $\mu H + 2J_1 - 2J_2$, $\mu H - 2J_1 - 2J_2$, $\mu H - 2J_2$ $\mu H - 2J_2$, $\mu H + 2J_1$, $\mu H - 2J_1$, μH, μH, $\mu H + 2J_1$, $\mu H - 2J_1$, μH, μH, $\mu H + 2J_1$, $\mu H - 2J_1$, μH, μH, $\mu H + 2J_1$, $\mu H - 2J_1$, μH, μH, $-\mu H + 2J_1 + 2J_2$, $-\mu H - 2J_1 + 2J_2$, $-\mu H + 2J_2$, $-\mu H + 2J_1 - 2J_2$, $-\mu H - 2J_1 - 2J_2$, $-\mu H - 2J_2$, $-\mu H - 2J_2$, $-\mu H - 2J_2$, $-\mu H + 2J_1$, $-\mu H - 2J_1$, $-\mu H$, $-\mu H$, $-\mu H + 2J_1$, $-\mu H - 2J_1$, $-\mu H$ and $-\mu H$.

Some of the energies are of course repeated. Similarly in three dimensions the arbitrary (l, m, n)th site will have energy given by

$$E_{lmn} = -\mu H\sigma_{lmn} - J_1\sigma_{lmn}\sigma_{l+1mn} - J_1\sigma_{lmn}\sigma_{l-1mn} - J_2\sigma_{lmn}\sigma_{lm+1n} - J_2\sigma_{lmn}\sigma_{lm-1n} - J_3\sigma_{lmn}\sigma_{lmn+1} - J_3\sigma_{lmn}\sigma_{lmn-1} \qquad \ldots (3)$$

There will be 128 $(= 2^7)$ energy values.

The total energy of the crystal will be given by $E = \sum_{l=1,\ m=1,\ n=1}^{l=L,\ m=M,\ n=N} E_{lmn}$

The average energy $\bar{E}$ will be however LMN times the average value $\bar{E}_{lmn}$.

Partition Function

The partition function is given by

$$Z = \Sigma\, e^{-\frac{E^i}{kT}} \qquad \dots (4)$$

where k is Boltzmann constant, T is absolute temperature and E^i is a possible energy value. Free energy is related to partition function by

$$F = -kT \ln Z \qquad \dots (5)$$

If F_{lmn} be free energy per site, total free energy will be given by

$$F = LMN\, F_{lmn} \qquad \dots (6)$$

Let Z_{lmn} be partition function per site.

$$F \quad = LMN\, F_{lmn} = -kT \ln Z$$

$$F_{lmn} = -\frac{kT}{LMN} \ln Z = -kT \ln (Z)^{\frac{1}{LMN}} \qquad \dots (7)$$

But

$$F_{lmn} = -kT \ln Z_{lmn} \qquad \dots (8)$$

So

$$Z_{lmn} = (Z)^{\frac{1}{LMN}} \quad \text{or} \quad Z = (Z_{lmn})^{LMN} \qquad \dots (9)$$

Let Z_{lmn} be given by $Z_{lmn} = \sum_i e^{-\frac{Ei}{kT}}$

$$= \Sigma\, e^{-\frac{E_{lmn}}{kT}(\sigma_{lmn},\, \sigma_{l+1mn},\, \sigma_{l-1mn},\, \sigma_{lm+1n},\, \sigma_{lm-1n},\, \sigma_{lmn+1},\, \sigma_{lmn-1})}; \qquad \dots (10)$$

$$\sigma_{lmn}, \sigma_{l+1mn}, \sigma_{l-1mn}, \sigma_{lm+1n}, \sigma_{lm-1n}, \sigma_{lmn+1}, \sigma_{lmn-1} = \pm 1$$

Thermodynamic Functions

The various thermodynamic functions are related to the free energy. Average energy E, average magnetic moment M in magnetic field H, spontaneous magnetization $(M)_{H=0}$, entropy S, specific heat C_V, susceptibility χ, spin average $< \sigma >$ and spin correlation $< \sigma\sigma' >$ are given by the following relations

$$E = -T^2 \frac{\partial}{\partial T}\left(\frac{F}{T}\right) \qquad \dots (11)$$

$$M = -\frac{\partial F}{\partial H}$$

$$(M)_{H=0} = -\left(\frac{\partial F}{\partial H}\right)_{H=0} \qquad \dots (12)$$

$$S = -\frac{\partial F}{\partial T} \qquad \ldots (13)$$

$$C_V = \left(\frac{\partial E}{\partial T}\right)_{H=0} \qquad \ldots (14)$$

$$\chi = \left(\frac{\partial M}{\partial H}\right)_{H=0} \qquad \ldots (15)$$

$$<\sigma> = <\sigma_{lmn}> = -\frac{1}{LMN\mu}\frac{\partial F}{\partial H} \qquad \ldots (16)$$

$$<\sigma\sigma'>_1 = <\sigma_{lmn}\sigma_{l+1mn}> = -\frac{1}{LMN}\frac{\partial F}{\partial J_1}$$

$$<\sigma\sigma'>_2 = <\sigma_{lmn}\sigma_{lm+1n}> = -\frac{1}{LMN}\frac{\partial F}{\partial J_2}$$

$$<\sigma\sigma'>_3 = <\sigma_{lmn}\sigma_{lmn+1}> = -\frac{1}{LMN}\frac{\partial F}{\partial J_3} \qquad \ldots (17)$$

Construction of Partition Function in one Dimension

We immediately get the partition function Z_l (figure 4)

$$Z_l = \sum_{\sigma_l, \sigma_{l+1}, \sigma_{l-1} = \pm 1} e^{-\frac{El}{kT}(\sigma_l, \sigma_l, \sigma_{l+1}, \sigma_l, \sigma_{l-1})}$$

$$= e^{\frac{\mu H - 2J_1}{kT}} + e^{\frac{\mu H - 2J_1}{kT}} + e^{\frac{-\mu H + 2J_1}{kT}} + e^{\frac{-\mu H - 2J_1}{kT}} + 2e^{\frac{\mu H}{kT}} + 2e^{\frac{-\mu H}{kT}}$$

$$= \left(e^{\frac{\mu H}{kT}} + e^{-\frac{\mu H}{kT}}\right)\left(e^{\frac{J_1}{kT}} + e^{-\frac{J_1}{kT}}\right)^2$$

$$= 8\text{ch}\,\frac{\mu H}{kT}\,\text{ch}^2\,\frac{J_1}{kT}\,. \qquad \ldots (18)$$

$$Z = 8^L\text{ch}^L\,\frac{\mu H}{kT}\,\text{ch}^{2L}\,\frac{J_1}{kT} \qquad \ldots (19)$$

PARTITION FUNCTION IN TWO DIMENSIONS

Easily we get partition function Z_{lm} (figure 5)

$$Z_{lm} = e^{\frac{\mu H+2J_1+2J_2}{kT}} + e^{\frac{\mu H-2J_1+2J_2}{kT}} + 2e^{\frac{\mu H+2J_2}{kT}} + e^{\frac{\mu H+2J_1-2J_2}{kT}}$$

$$+e^{\frac{\mu H-2J_1-2J_2}{kT}} + 2e^{\frac{\mu H-2J_2}{kT}} + 2e^{\frac{\mu H+2J_1}{kT}} + 2e^{\frac{\mu H-2J_1}{kT}} + 4e^{\frac{\mu H}{kT}}$$

$$+4e^{\frac{-\mu H}{kT}} + e^{\frac{-\mu H+2J_1+2J_2}{kT}} + e^{\frac{-\mu H-2J_1+2J_2}{kT}} + e^{\frac{-\mu H+2J_1-2J_2}{kT}}$$

$$+e^{\frac{-\mu H-2J_1-2J_2}{kT}} + 2e^{\frac{-\mu H+2J_1}{kT}} + 2e^{\frac{-\mu H-2J_1}{kT}} + 2e^{\frac{-\mu H+2J_2}{kT}}$$

$$+2e^{\frac{-\mu H-2J_2}{kT}}$$

$$= \left(e^{\frac{\mu H}{kT}} + e^{-\frac{\mu H}{kT}} \right) \left(e^{\frac{J_1}{kT}} + e^{-\frac{J_1}{kT}} \right)^2 \left(e^{\frac{J_2}{kT}} + e^{-\frac{J_2}{kT}} \right)^2$$

$$= 32 \operatorname{ch} \frac{\mu H}{kT} \operatorname{ch}^2 \frac{J_1}{kT} \operatorname{ch}^2 \frac{J_2}{kT} \qquad \dots (20)$$

$$Z = 32^{LM} \operatorname{ch}^{LM} \frac{\mu H}{kT} \operatorname{ch}^{2LM} \frac{J_1}{kT} \operatorname{ch}^{2LM} \frac{J_2}{kT} \qquad \dots (21)$$

PARTITION FUNCTION IN THREE DIMENSIONS

In a similar manner we get partition function for the three dimensional case.

$$Z_{lmn} = \left(e^{\frac{\mu H}{kT}} + e^{-\frac{\mu H}{kT}} \right) \left(e^{\frac{J_1}{kT}} + e^{-\frac{J_1}{kT}} \right)^2 \left(e^{\frac{J_2}{kT}} + e^{-\frac{J_2}{kT}} \right)^2 \left(e^{\frac{J_3}{kT}} + e^{-\frac{J_3}{kT}} \right)^2$$

$$128 \operatorname{ch} \frac{\mu H}{kT} \operatorname{ch}^2 \frac{J_1}{kT} \operatorname{ch}^2 \frac{J_2}{kT} \operatorname{ch}^2 \frac{J_3}{kT} \qquad \dots (22)$$

$$Z = 128^{LMN} \operatorname{ch}^{LMN} \frac{\mu H}{kT} \operatorname{ch}^{2LMN} \frac{J_1}{kT} \operatorname{ch}^{2LMN} \frac{J_2}{kT} \operatorname{ch}^{2LMN} \frac{J_3}{kT} \qquad \dots (23)$$

We easily observe that by putting $N = 1$ and $J_3 = 0$, free energy for the two dimensional case follows from that of the three dimensional case and by putting $M = N = 1$ and $J_2 = J_3 = 0$ (or by putting $M = 1$ and $J_2 = 0$ in the two dimensional case) in the three dimensional case we get free energy of the one dimensional case. It is better if $L \geqslant 3$, $M \geqslant 3$ and $N \geqslant 3$, otherwise we cannot get two neighbours inside a crystal. Normally L, M and N are large. For sites in extreme position, one of the neighbours is in the neighbouring crystal. If $L = 2$ say, $\sigma_{2m}\sigma_{3m} = \sigma_{2m}\sigma_{1m}$ in two dimensions. A crystal can also be possible with $L < 3$, $M < 3$ and $N < 3$.

Results

One finds that free energy comes out to be a continuous function of temperature and the derivatives of free energy are also continuous. There is no discontinuity in any order derivative of the thermodynamic potential and so in this model a transition temperature is not obtained and also not spontaneous magnetization. The earlier workers do not get a transition temperature and spontaneous magnetization is one dimension, but they get them in two dimensions. In none of our calculations, either in one, two or three dimensional, there is a transition temperature or spontaneous magnetization. This is however not surprising because one dimensional calculations are expected to behave similar to the two dimensional calculations. The experimental results are shown qualitatively in figures 4–8 and theoretical values given qualitatively in figures 9–20.

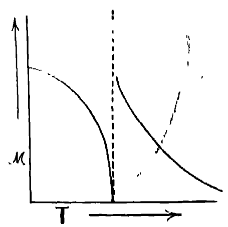


Fig. 4

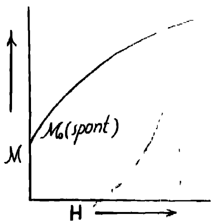
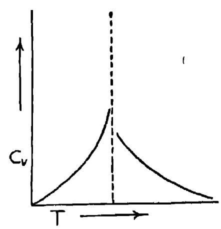


Fig. 5



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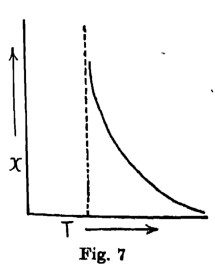

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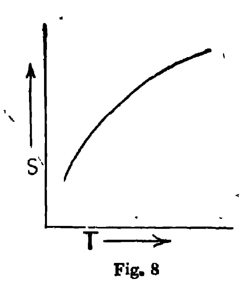

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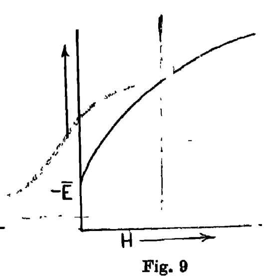

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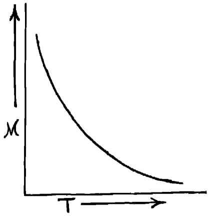


Fig. 10

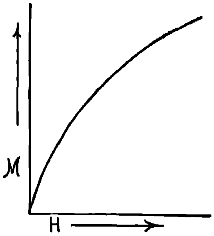
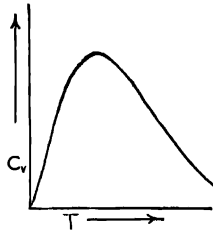


Fig. 11



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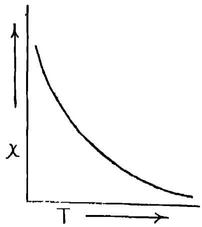

Fig. 13

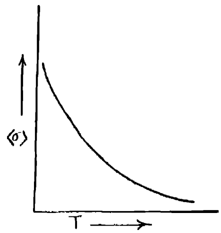

Fig. 14

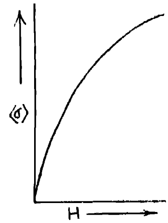

Fig. 15

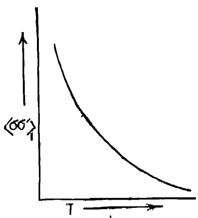

Fig. 16

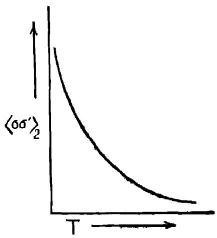

Fig. 17

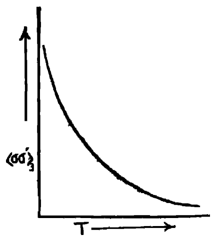

Fig. 18

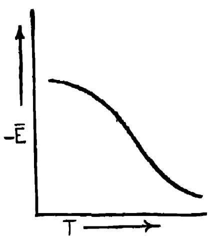

Fig. 19

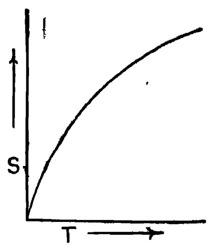

Fig. 20

Conclusion

We have the following expressions for partition functions in various dimensions

1 dimension $$Z = 8^L \mathrm{ch}^L \frac{\mu H}{kT} \mathrm{ch}^{2L} \frac{J_1}{kT} \quad \dots (19)$$

2 dimensions $$Z = 32^{LM} \mathrm{ch}^{LM} \frac{\mu H}{kT} \mathrm{ch}^{2LM} \frac{J_1}{kT} \mathrm{ch}^{2LM} \frac{J_2}{kT} \quad \dots (21)$$

3 dimensions $$Z = 128^{LMN} \mathrm{ch}^{LMN} \frac{\mu H}{kT} \mathrm{ch}^{2LMN} \frac{J_1}{kT} \mathrm{ch}^{2LMN} \frac{J_2}{kT} \mathrm{ch}^{2LMN} \frac{J_3}{kT} \quad \dots (23)$$

If we take

$$Z = \left\{ \sum_{\dots,\, \sigma_{lmn} = \pm 1,} e^{\frac{1}{kT}(\mu H \sigma_{lmn} + 2J_1 \sigma_{lmn}\sigma_{l+1mn} + 2J_2 \sigma_{lmn}\sigma_{lm+1n} + 2J_3 \sigma_{lmn}\sigma_{lmn+1})} \right\}^{LMN} \quad \dots (24)$$

the result will be

$$Z = 16^{LMN} \mathrm{ch}^{LMN} \frac{\mu H}{kT} \mathrm{ch}^{LMN} \frac{2J_1}{kT} \mathrm{ch}^{LMN} \frac{2J_2}{kT} \mathrm{ch}^{LMN} \frac{2J_3}{kT} \quad \dots (25)$$

which will not give any qualitative difference.

One may not like to agree with the fact that

$$Z = \left(\sum_{\dots,\sigma_{lmn} = \pm 1, \dots} e^{-\frac{E_{lmn}}{kT}} \right)^{LMN} \quad \dots (26)\text{-I}$$

but one may say

$$Z = \sum_{\dots,\, \sigma_{lmn} = \pm 1, \dots} e^{-\sum_{l=1,\, m=1,\, n=1}^{l=L,\, m=M,\, n=N} \frac{E_{lmn}}{kT}}$$

$$= \sum_{\dots,\, \sigma_{lmn} = \pm 1, \dots} e^{\frac{1}{kT} \sum_{l=1,\, m=1,\, n=1}^{l=L,\, m=M,\, n=N} (\mu H \sigma_{lmn} + 2J_1 \sigma_{lmn}\sigma_{l+1mn} + 2J_{-2} \sigma_{lmn}\sigma_{lm+1} + 2J_3 \sigma_{lmn}\sigma_{lmn+1})} \quad \dots (27)\text{-II}$$

It may be pointed out that the expression II is identical with I for free spins (*i e.* if $J_1 = J_2 = J_3 = 0$). However the expression II is a part of the expression I, so there will be no qualitative difference in thermodynamic results. For a ferromagnetic substance at low temperatures with the condition $\sigma = \pm 1$, there will be very few spins that will align against the magnetic field with $\sigma = -1$ and most of the spins will align in the direction of the magnetic field with $\sigma = +1$.

The two expressions will differ very little. It may be pointed out that considering the two dimensional cases $L = 2$, $M = 2$, $N = 1$ (16 terms), $L = 3$, $M = 2$, $N = 1$ (64 terms) and $L = 3$, $M = 3$, $N = 1$ (512 terms) as examples, we have evaluated the exact partition function according to expression II. We have calculated free energy, specific heat, magnetization etc. and have found that there is no spontaneous magnetization or discontinuity in the specific heat in the two dimensions. It would appear that the results of Onsager (1944) and Yang (1952) are not so reliable.

The author is thankful to the Ministry of Scientific Research and Cultural Affairs, Government of India, for the award of a Senior Research Scholarship for carrying on this work. He is grateful to Prof. F. C. Auluck, D.Sc., F.N.A. for suggesting the problem.

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